Trifluprомazine M (hydroxy-), acetylated

Inchi: InChI=1S/C20H21F3N2O2S/c1-13(26)27-15-6-7-16-19(12-15)28-18-8-5-14(20(21,22)23)
InchiKey: CTTSKTQYYQVSNS-UHFFFAOYSA-N
Formula: C20H21F3N2O2S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccc(C(F)(F)F)cc1N2CCCN(C)C
Mol. weight [g/mol]: 410.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.50		Crippen Method
logp	5.185		Crippen Method
mcvol	283.340	ml/mol	McGowan Method
rinpol	2720.00		NIST Webbook
rinpol	2720.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R314568&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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